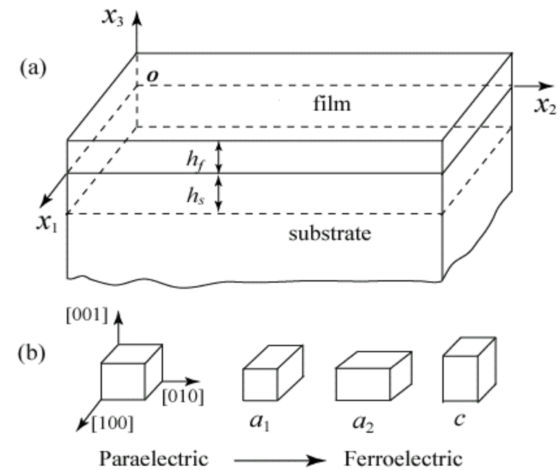
# Microstructure Evolution in Solids with External Constraints and Defects

Long-Qing Chen, Penn State University

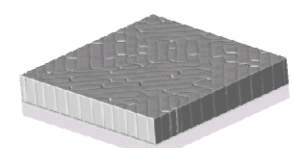
DMR Award#DMR-0122638

Ferroelectric thin films have potential applications in many electronic and electro-optical devices, including nonvolatile memories, sensors, surface acoustic wave substrates, optical waveguides, optical memories and displays. One of the factors that control the physical properties of ferroelectric thin films is their domain structure within which regions of uniform electric polarization separated by domain-walls.

Using a combination of materials theory and the fundamentals of mechanics and electrostatics, we developed a computer simulation model that may be used to predict the ferroelectric domain structures under different thin film growth temperatures and types of substrate. As an example, the model is applied to $PbTiO_3$ thin films on a cubic substrate, and a domain stability map is constructed, which will allow one to design a domain structure by choosing the appropriate temperature and substrate constraint.




24% a ($a_1$+$a_2$) domains under a compressive strain



100% a-domains under a large tensile misfit strain

Fig. 1a shows the computational cell consisting of a single crystal film on a thick substrate. The film undergoes a phase transformation from a cubic paraelectric to a tetragonal ferroelectric phase which has three orientational domains (Fig.1b) labeled as $a_1$, $a_2$ (tetragonal axes parallel to the film surface) and c (tetragonal axes normal to the film surface. Different substrate constraints result in dramatically different domain structures shown in the lower part of Fig. 1.

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Educational:
1 high school student (this summer)
1 undergraduate (working on B.S. thesis)
1 grad student
1 post-doc

Brief summary of outreach activities:

- the PI taught a short course on introduction to phase-field simulation to scientists and engineers from industry, national labs and universities (May, 2002)
- the PI is mentoring a high school student this summer for learning parallel computing and building a linux cluster
- the PI helped with the Engineering Open House (March 2002) and the EMEX open house (April 2002) for recruiting undergraduate students to the Department of Materials Science
- The PI participated in the Douglass Science Institute Program Series at Rutgers University for 9th-12th grade girls (see figure 2)

Figure 2. The PI participated in the Douglass Science Institute Program Series at Rutgers University for 9th-12th grade girls (November 2001 and December 2002). In the two workshops, the PI discussed the energetics of soap bubbles and allow students to explore these energetics with a hands-on activity in which the students made rafts of bubbles and watched what happens when the bubbles agglomerate. These interactions are relevant to grain morphology and grain growth in solids, but involve soap bubbles with which the students are bound to be familiar. This figure shows 5 students working together to build babble raft. (This activity is also associated with the NIRT project DMR-0103354)